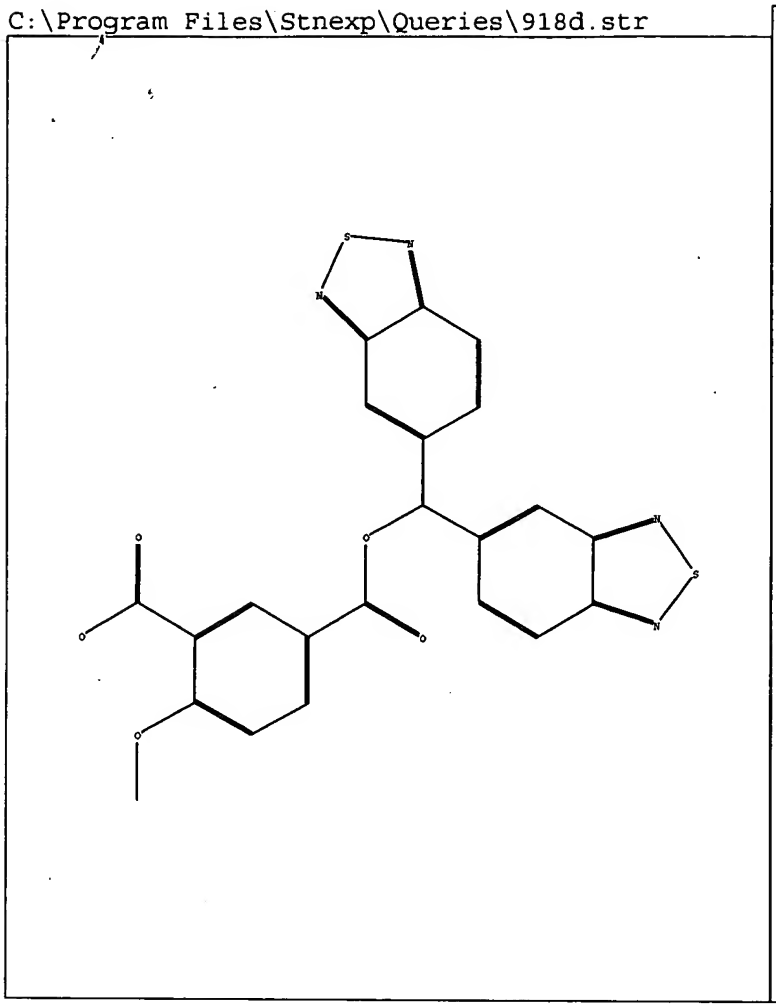
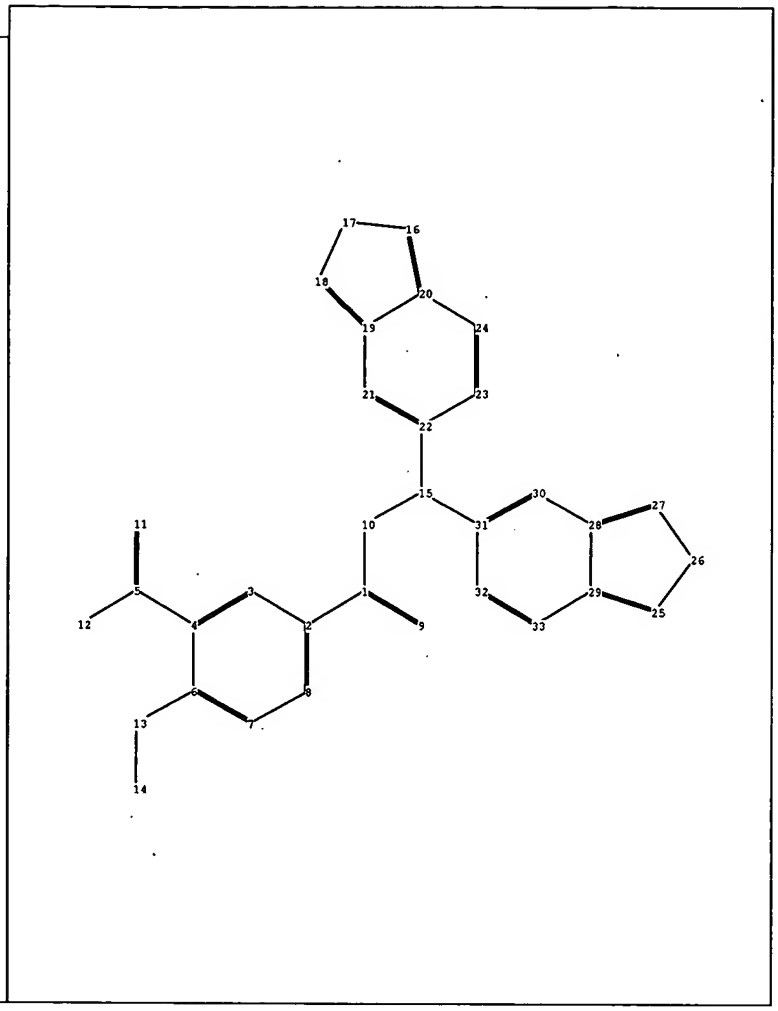
C:\Program Files\Stnexp\Queries\918d.str

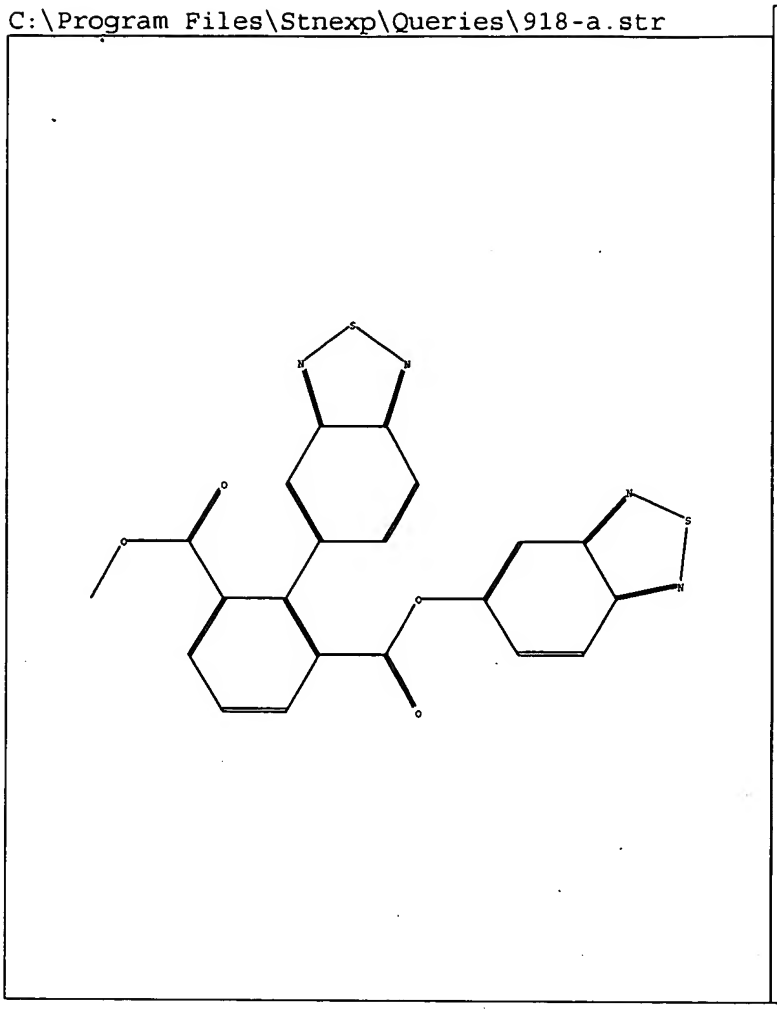


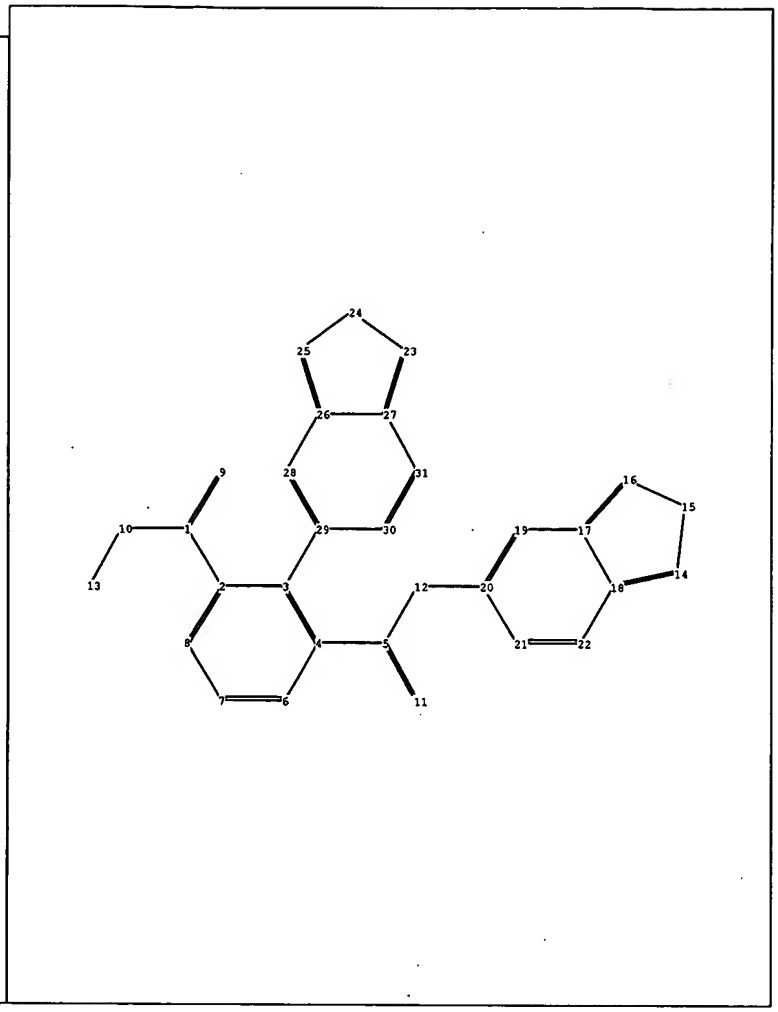


ring nodes :
2 3 4 6 7 8 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33
ring/chain nodes :
1 5 9 10 11 12 13 14 15
ring/chain bonds :
1-2 1-9 1-10 4-5 5-11 5-12 6-13 10-15 13-14 15-22 15-31
ring bonds :
2-3 2-8 3-4 4-6 6-7 7-8 16-17 16-20 17-18 18-19 19-20 19-21 20-24 21-22
22-23 23-24 25-26 25-29 26-27 27-28 28-29 28-30 29-33 30-31 31-32 32-33
exact/norm bonds :
1-2 4-5 15-22 15-31
exact bonds :
1-9 1-10 5-11 5-12 6-13 10-15 13-14 16-17 16-20 17-18 18-19 19-20 19-21
20-24 21-22 22-23 23-24 25-26 25-29 26-27 27-28 28-29 28-30 29-33 30-31 31-32
32-33
normalized bonds :
2-3 2-8 3-4 4-6 6-7 7-8

Match level :
1:CLASS 2:Atom 3:Atom 4:Atom 5:CLASS 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom

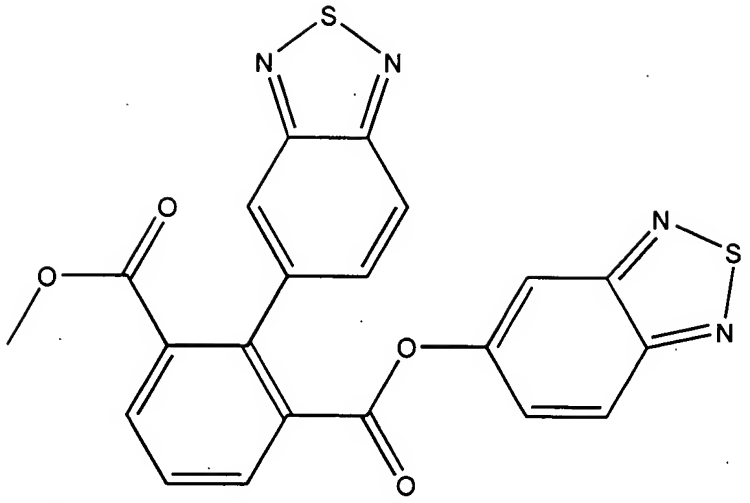
C:\Program Files\Stnexp\Queries\918-a.str



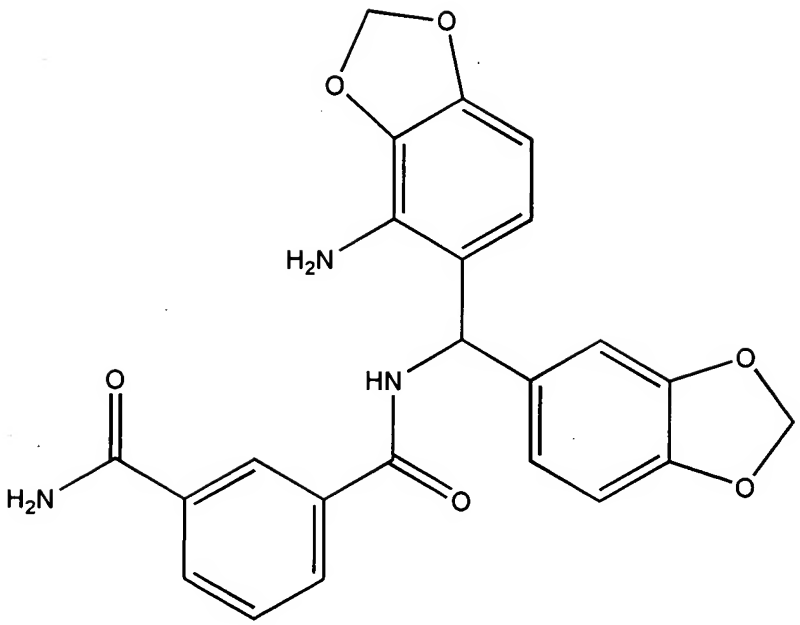


ring nodes :
2 3 4 6 7 8 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
ring/chain nodes :
1 5 9 10 11 12 13
ring/chain bonds :
1-2 1-9 1-10 3-29 4-5 5-11 5-12 10-13 12-20
ring bonds :
2-3 2-8 3-4 4-6 6-7 7-8 14-15 14-18 15-16 16-17 17-18 17-19 18-22 19-20
20-21 21-22 23-24 23-27 24-25 25-26 26-27 26-28 27-31 28-29 29-30 30-31
exact/norm bonds :
1-2 3-29 4-5
exact bonds :
1-9 1-10 5-11 5-12 10-13 12-20 14-15 14-18 15-16 16-17 17-18 17-19 18-22
19-20 20-21 21-22 23-24 23-27 24-25 25-26 26-27 26-28 27-31 28-29 29-30 30-31
normalized bonds :
2-3 2-8 3-4 4-6 6-7 7-8

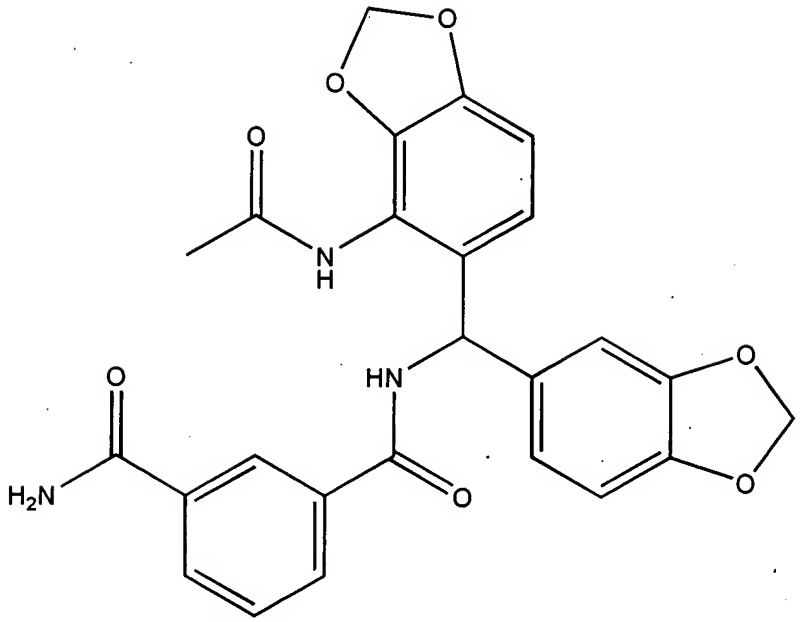
Match level :
1:CLASS 2:Atom 3:Atom 4:Atom 5:CLASS 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
30:Atom 31:Atom



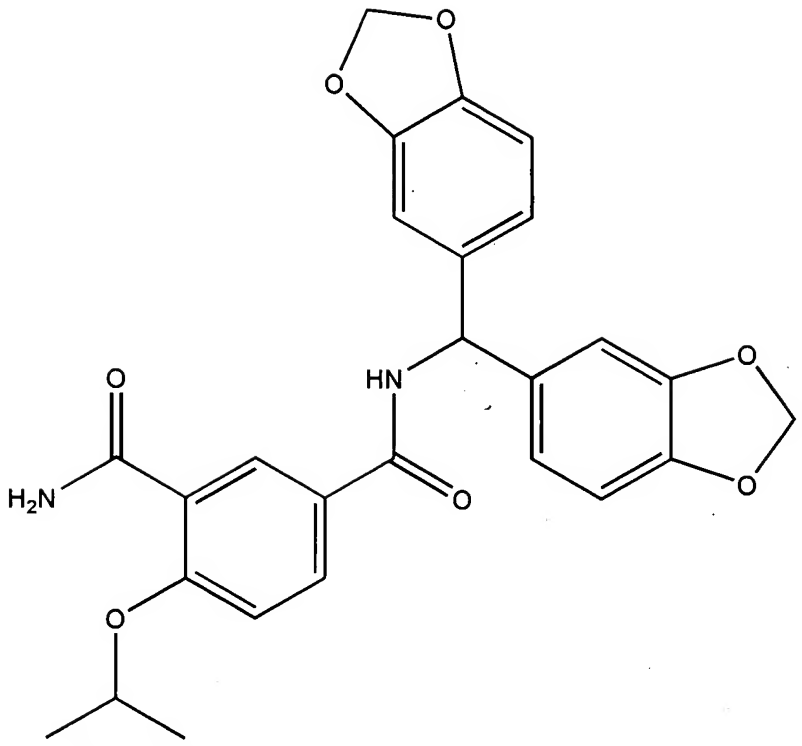
isophthalic acid di-(2,1,3-benzothiadiazol-5-yl) methyl ester



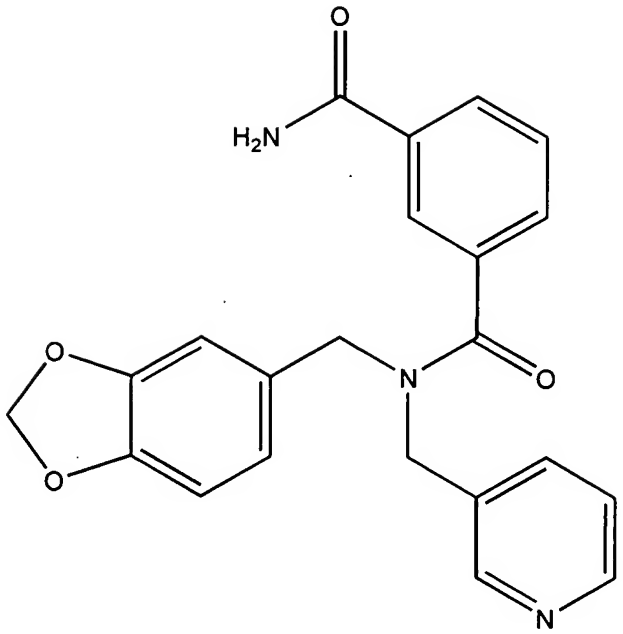
4-amino-bis-1,3-benzodioxol-5-ylmethyl-isophthalamide



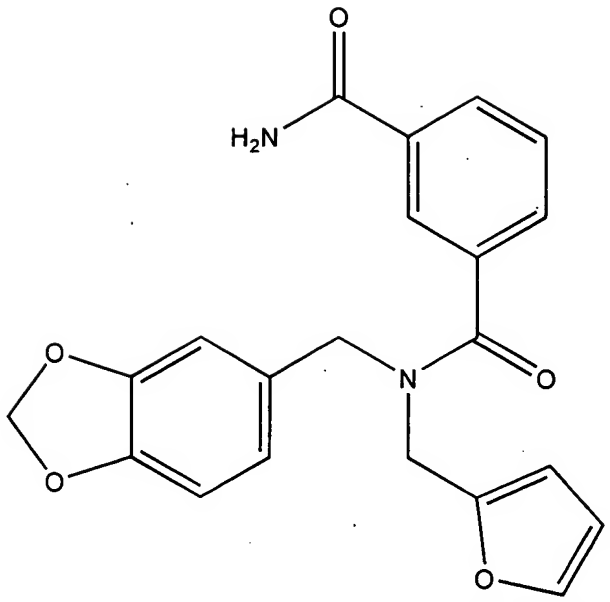
4-acetylamino-bis-1,3-benzodioxol-5-ylmethyl-isophthalamide



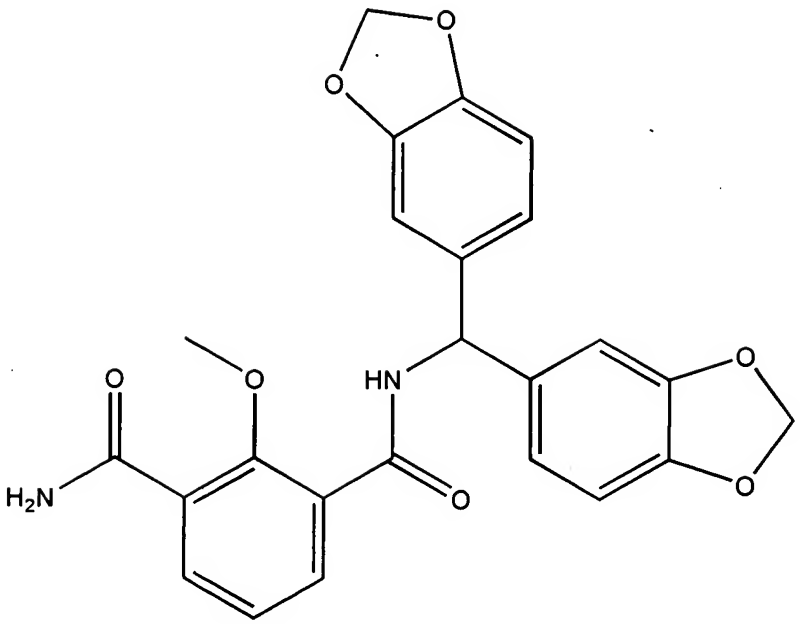
bis-1,3-benzodioxol-5-ylmethyl-4-isopropoxy-isophthalamide



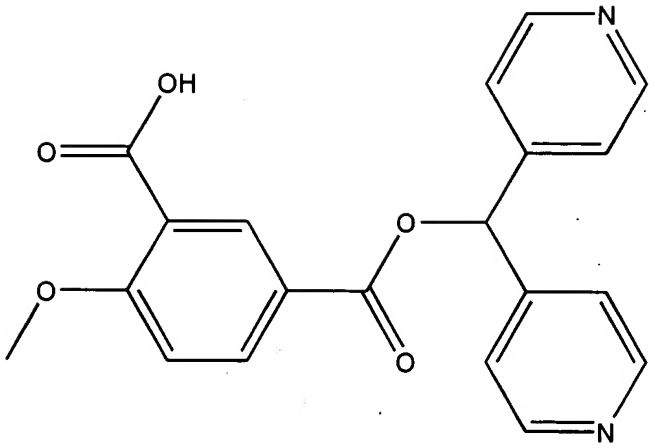
1,3-benzodioxol-5-ylmethyl-pyridin-3-ylmethyl-isophthalamide



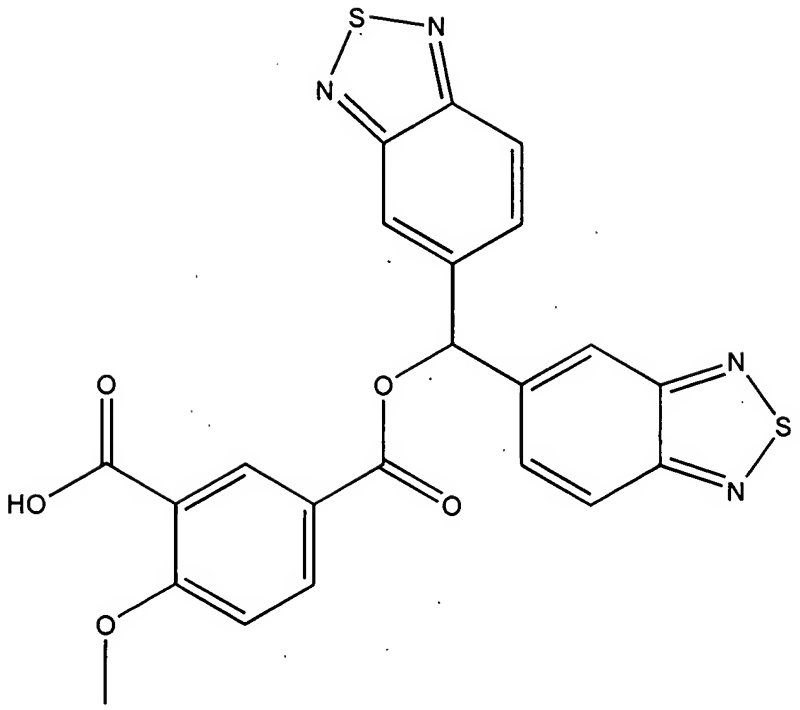
1,3-benzodioxol-5-ylmethyl-furan-2-ylmethyl-isophthalamide



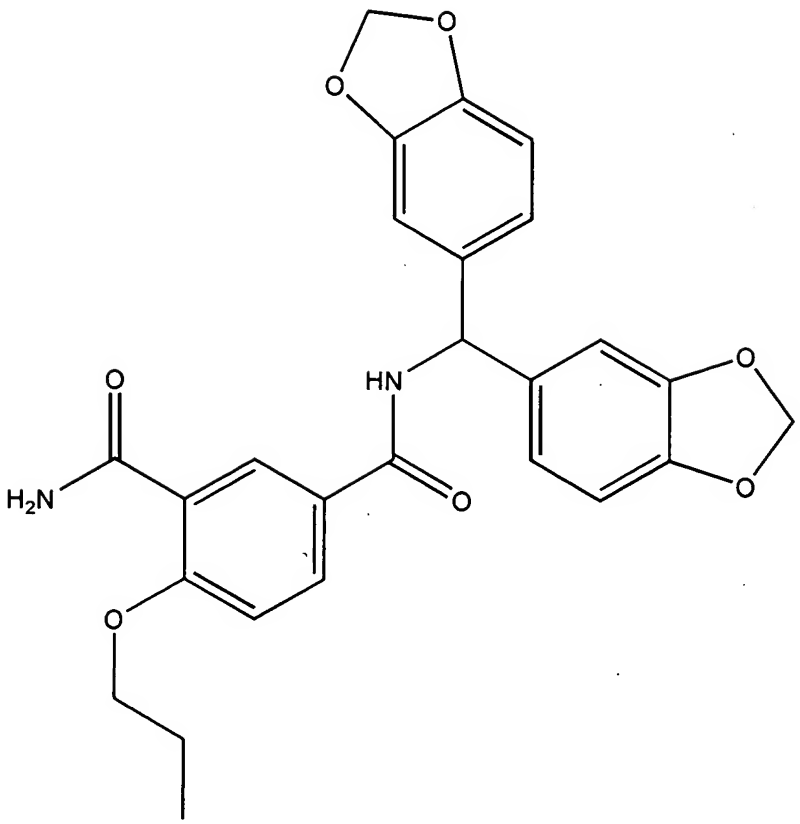
bis-1,3-benzodioxol-5-ylmethyl-methoxy-isophthalamide



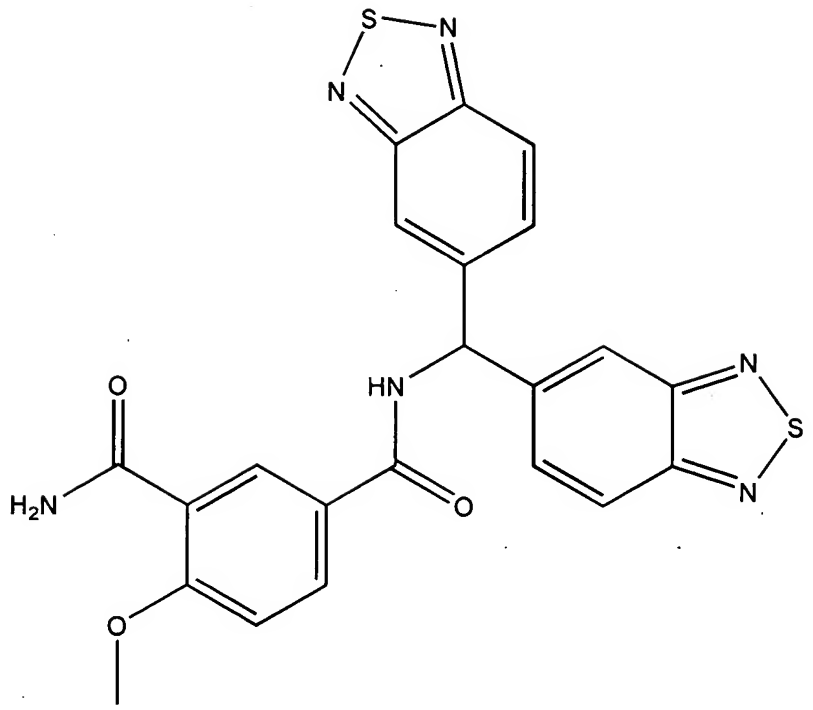
4-methoxy-isophthalic acid dipyridin-4-ylmethyl ester



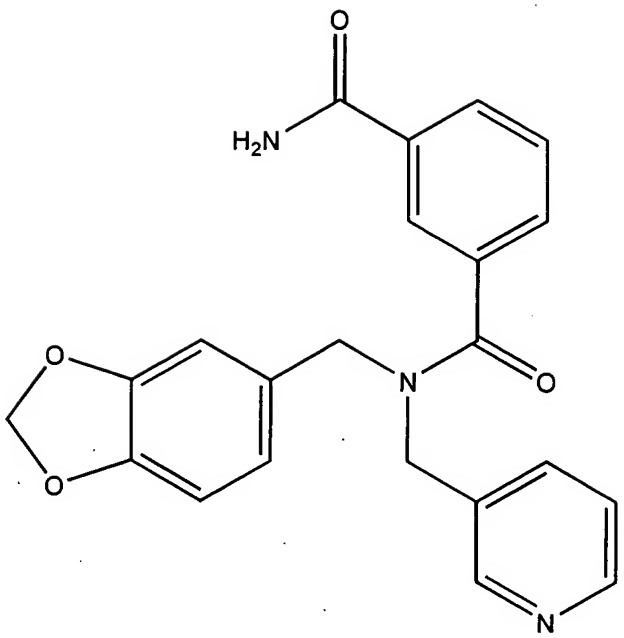
4-methoxy-isophthalic acid di-2,1,3-benzothiadiazol-5-ylmethyl ester



bis-1,3-benzodioxol-5-ylmethyl-4-propoxy-isophthalamide



bis-2,1,3-benzothiadiazol-5-ylmethyl-4-methoxy-isophthalamide



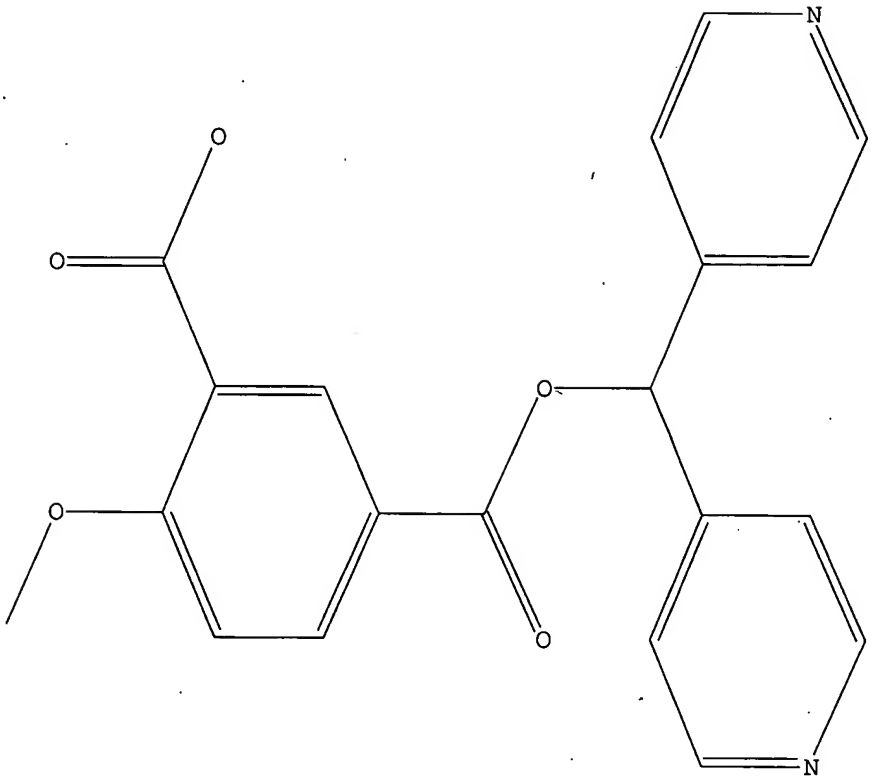
1,3-benzodioxol-5-ylmethyl-pyridin-3-ylmethyl-isophthalamide

```
Uploading C:\Program Files\Stnexp\Queries\918d.str

L17     STRUCTURE UPLOADED

=> d
L17 HAS NO ANSWERS
L17             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s 17
L18     636092 17

=> s l17
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 15:59:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     16 TO ITERATE

100.0% PROCESSED      16 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           80 TO      560
PROJECTED ANSWERS:               0 TO        0

L19           0 SEA SSS SAM L17


L20          0 L19

=> s l17 full
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 15:59:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    361 TO ITERATE

100.0% PROCESSED     361 ITERATIONS                               0 ANSWERS
SEARCH TIME: 00.00.01

L21           0 SEA SSS FUL L17


L22          0 L21
```

```
str

L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 15:47:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     16 TO ITERATE

100.0% PROCESSED      16 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           80 TO      560
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1



L3           0 L2

=> s l1 full
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 15:47:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    361 TO ITERATE

100.0% PROCESSED     361 ITERATIONS                               0 ANSWERS
SEARCH TIME: 00.00.01

L4            0 SEA SSS FUL L1



L5           0 L4

=>
Uploading C:\Program Files\Stnexp\Queries\918-b.str
```

L6 STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l6
REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:49:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1287 TO ITERATE

77.7% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 23588 TO 27892
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

L8 0 L7

=> s l6 full
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:49:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 26222 TO ITERATE

100.0% PROCESSED 26222 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

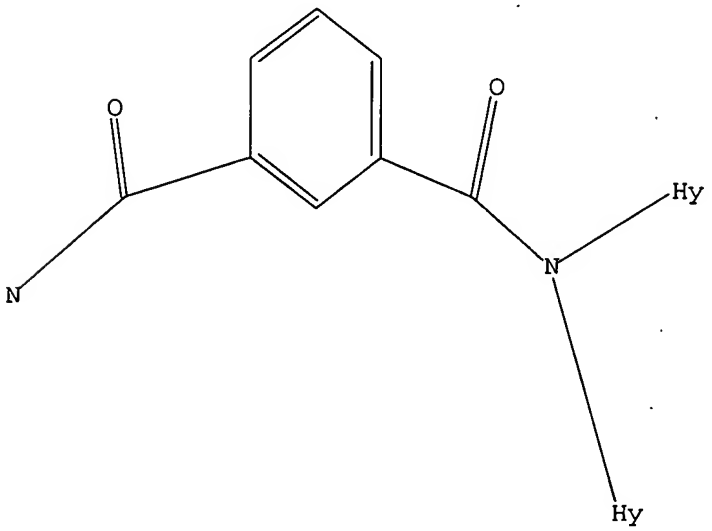
L9 0 SEA SSS FUL L6

L10 0 L9

=>
Uploading C:\Program Files\Stnexp\Queries\918c.str

L11 STRUCTURE UPLOADED

=> d
L11 HAS NO ANSWERS
L11 STR



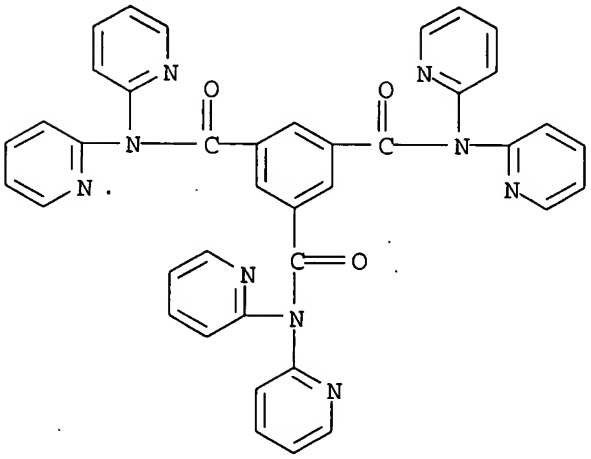
Structure attributes must be viewed using STN Express query preparation.

```
=> s l11
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 15:54:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3453 TO ITERATE

 29.0% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        65536 TO    72584
PROJECTED ANSWERS:               0 TO        0

L12           0 SEA SSS SAM L11


L13           0 L12

=> s l11 full
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 15:54:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  68618 TO ITERATE

100.0% PROCESSED   68618 ITERATIONS                               2 ANSWERS
SEARCH TIME: 00.00.01

L14           2 SEA SSS FUL L11


L15           2 L14

=> s l15 and  py<2001
      20649979 PY<2001
L16           0 L15 AND  PY<2001

=> d l15 1-2 ibib abs hitstr

L15  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2003:263059  CAPLUS
DOCUMENT NUMBER:          139:110540
TITLE:                    Dinuclear copper(II) complexes with different bridging
                          connectors
AUTHOR(S):                Huang, W.; Hu, D.; Gou, S.; Qian, H.; Fun, H.-K.; Raj,
                          S. S. S.; Meng, Q.
```

CORPORATE SOURCE: State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2003), 649(3), 269-278
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:110540

AB One novel triply-bridged dicopper(II) complex formulated as [Cu2(dpa)2(μ-Cl)(μ-OH)(μ-HCOO)]·(ClO4) (1, dpa = 2,2'-dipyridylamine) and two terephthalate anion bridged 2,2'-bipyridine (2,2'-bpy) dicopper(II) complexes of [Cu2(2,2'-bpy)4(μ-terephthalate)]·(NO3)2 (2) and [Cu2(2,2'-bpy)4(μ-terephthalate)]·(terephthalate) (3), resp., were synthesized and characterized by IR and electrospray mass spectra as well as x-ray single-crystal determination Thermal properties of all compds. were studied.

IT **557767-01-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant for preparation of copper(II) chloro hydroxo formato triply-bridged dipyridylamine dinuclear complex)
RN 557767-01-8 CAPLUS
CN 1,3,5-Benzenetricarboxamide, N,N,N',N',N'',N''-hexa-2-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:146239 CAPLUS
DOCUMENT NUMBER: 136:334309
TITLE: Synthesis and molecular structure of N,N'-bis(2,2'-dipyridyl)isophthaloylamide as well as its reaction with copper(II) perchlorate
AUTHOR(S): Hu, Dahua; Huang, Wei; Gou, Shaohua; Chantrapromma, Suchada; Fun, Hoong-Kun; Xu, Yan
CORPORATE SOURCE: State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China
SOURCE: Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (2002), 32(1), 127-141
CODEN: SRIMCN; ISSN: 0094-5714
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:334309

AB N,N'-Bis(2,2'-dipyridyl)isophthaloylamide (1) and its coordination product with a copper(II) ion, bis(2,2'-dipyridylamine)copper(II) diperchlorate (2), were prepared and spectroscopically characterized. X-ray structural results indicate that 1 has the expected configuration derived from the reaction between isophthaloyl dichloride and 2,2'-dipyridylamine (dpa) at a ratio of 1:2; while in complex 2, the copper atom is only coordinated to two dpa groups rather than the ligand 1 as anticipated. This known complex has a distorted tetrahedral configuration with two pyridine rings of each dpa moiety nearly coplanar to each other, and the dihedral angle of the two coordinating dpa ligands is 56.8°. Also the crystal structural study revealed that two-dimensional networks are formed by weak H-bonding interactions and π-π stacking interactions in both 1 and 2.

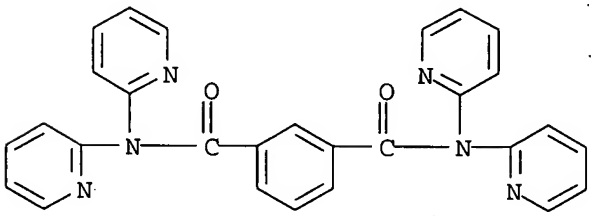
IT **325823-56-1P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and crystal and mol. structure and reaction with copper(II) perchlorate to give dipyridylamine complex)

RN 325823-56-1 CAPLUS

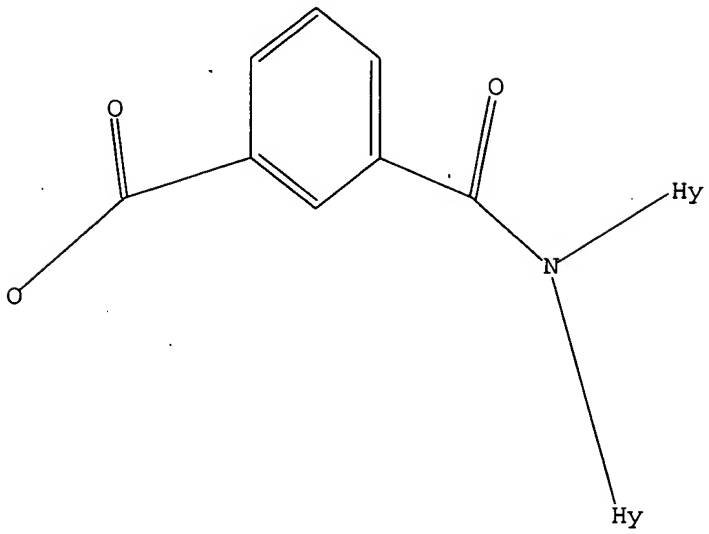
CN 1,3-Benzenedicarboxamide, N,N,N',N'-tetra-2-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 STRUCTURE UPLOADED

=> d
L23 HAS NO ANSWERS
L23 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l23
REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 16:04:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9567 TO ITERATE

10.5% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 185479 TO 197201
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

L25 0 L24

=> s l23 full
REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 16:04:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 191427 TO ITERATE

100.0% PROCESSED 191427 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

L26 0 SEA SSS FUL L23

L27 0 L26

=>